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Numerical investigation on the effect of reactivity gradient in an RCCI engine fueled with gasoline and diesel

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ABSTRACT

The reactivity controlled compression ignition (RCCI), which belongs to dual fuel mode (DFM) combustion has been considered as a promising way to achieve high fuel conversion efficiency and low emissions. By this strategy, a fuel reactivity gradient is formed in the combustion chamber which offers the probability of controlling combustion phasing. In this study, the role of fuel reactivity gradient was examined numerically by comparing a DFM (i.e., RCCI) combustion with other hypothetical cases under one specific load condition. Firstly, a chemical reaction mechanism was developed aiming at a modelling study on dual fuel and blend fuel combustion in internal combustion (IC) engines fueled by gasoline/diesel and gasoline/biodiesel. Ignition delays were validated for 100% diesel, 100% gasoline and 100% biodiesel under 102 conditions in total. Subsequently, the validated reaction mechanism which consists of 107 species and 425 reactions was implemented in coupled KIVA4-CHEMKIN code. Three dimensional validations were further conducted under 3 conditions including pure diesel combustion, and gasoline/diesel DFM combustion with both single and double injection strategies in the engine. To investigate the fuel reactivity gradient, the gasoline/diesel DFM combustion with single injection was compared with other three hypothetical cases, one of which was DFM without fuel reactivity gradient, two were the blend fuel mode but with different start of injection (SOI) timings. The results showed that the fuel reactivity gradient could retard the ignition timing, reduce heat release rate, and ease peak pressure rise rate. In addition, low levels of NO_x and soot emissions were observed for the DFM combustion. The gasoline/biodiesel reaction mechanism will be employed in future work.

1. Introduction

The Industrial Revolution was a turning point in history which brought about large scale manufacturing and industrial operations. It also boosted the development of diesel engines; gradually diesel engines have been widely used in many areas such as on-road and off-road vehicles, marine ships and rail vehicles due to its high efficiency. However, the side effects, such as air pollution, aroused the attention of the government and the public. Legislative actions were taken to prevent air quality from deteriorating. The regulated pollutants from vehicles include carbon monoxide (CO), nitrogen oxides (NO_x), hydrocarbons (HC) and particulate matter (PM) [1], among which, NO_x and PM (including soot) emissions are main pollutions coming from diesel engines.

Though the use of aftertreatment system could achieve a low level of NO_x and soot emissions to fulfil the requirements of the regulations, the cost would become a major concern. Therefore, an economical way to curbing exhaust emissions is to develop an advanced in-cylinder combustion technique to reduce NO_x and soot. In the late 1990s, homogeneous charge compression ignition (HCCI) technique was proposed to reduce NO_x and soot simultaneously. The fuel is injected through port with air in HCCI mode, and Low NO_x and soot have been observed from low to medium loads. However, due to the chemical kinetic controlled heat release rate, HCCI technique faces unacceptable high noise and difficulties in controlling combustion phasing when the engines operating at high loads [2]. Inagaki et al. [3] studied HCCI and dual-fuel premixed compression ignition (PCI) modes in 2006. In dual fuel mode (DFM), one fuel with high volatility is injected through port and another fuel is directly injected into cylinder. The results showed that the stratification of ignitability in dual-fuel PCI engine could ease the heat release rate (HRR); thereby, higher load could be achieved even without exhaust gas recirculation (EGR) compared to HCCI mode. Based on above observations, Kokjohn et al. [4] found the optimized parameters (e.g., fuel combination, injection

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timing, injection duration, etc.) for both 6 bar and 11 bar IMEP loads by a multi-objective genetic algorithm; hence, the levels of NO_x and soot emissions were below the 2010 standard regulations in US while achieving 50% thermal efficiency. This finding implies that such a dual-fuel PCI engine promises a high thermal efficiency and low NO_x and soot emissions over a wide range of load conditions. Consequently, this regime is named as reactivity controlled compression ignition (RCCI) combustion because the in-cylinder combustion phasing is essentially controlled by fuel reactivity [5]. Some investigations on DFM combustion have been conducted swiftly [6–8]. Most recently, Benajes et al. [9] experimentally studied the effects of port-injected gasoline, gasoline/diesel blend ratio and start of injection (SOI) timing at light load condition of DFM combustion. The results showed that the factors could adjust the fuel reactivity in cylinder properly and subsequently achieve low NO_x and soot emissions. Desantes et al. [10] studied a gasoline/diesel fueled RCCI dual fuel engine and improved its combustion efficiency by combining the effects of in-cylinder gas temperature and oxygen concentration respectively with in-cylinder fuel blending. Li et al. [11] implemented a statistical approach to inspect the role of six factors (i.e., first SOI timing, the first injection duration, the second SOI timing, the second injection duration, the diesel mass fraction in the first injection and the ratio of natural gas to total air) and the interactions among them in a modelled natural gas/diesel fueled DFM engine. The results indicated the adoption of port-injected fuel plays a notable role in improving the performance and reducing emissions in a DFM combustion engine.

Ma et al. [12] experimentally investigated the influence of both single and double injection strategies with various injection timings on a gasoline/diesel dual fuel engine. Comparisons were made among four injection scenarios namely E-single (early injection timing of single), L-single (late injection timing of single), E-SOI2 (early second injection timing of double) and L-SOI2 (late second injection timing of double). It was found that the combustion characteristics of E-single with high gasoline percentage behaved more like HCCI combustion. As for the double injection strategy, the first diesel injection determined the reactivity of mixture; the second injection of diesel played a larger role in the formation of reactivity of stratification. Yang et al. [13,14] carried out the study on a gasoline/diesel fueled engine to compare the E-single, L-single and blend fuel mode (BFM) by experimental and numerical methods. Both E-single, L-single modes could be characterized into DFM. Their results showed that the maximum pressure rise rate (PRR) of BFM was higher than that of DFM. In another experimental comparative study between gasoline/diesel DFM and BFM carried out by Yu et al. [15], it was found that increase in gasoline ratio could significantly affect the ignition delay on BFM, not on DFM. Later, they achieved three DFM combustion scenarios namely fast single-stage combustion (FSC), two-stage combustion (TSC) and slow single-stage combustion (SSC) by adjusting the air–fuel ratio in a gasoline/diesel fueled engine [16]. It was found that TSC scenario was beneficial for extending to high load condition; also, the NO_x and soot emissions could be reduced by EGR.

Meanwhile, energy crisis is prompting researchers looking for alternative fuels in IC engines. Therefore, except for the investigations on DFM combustion fueled with gasoline/diesel, some studies focused on alternative fuels such as methanol [6,17,18], ethanol [19–21] and natural gas [22,23] as the port fuel substitutes in DFM. However, the directly injected fuel in DFM was still diesel which belongs to conventional fuel. Biodiesel, a kind of renewable fuel, has a great potential to substitute petroleum based diesel fuel. According to the previous study of our group [24], biodiesel characterizes a higher cetane number (CN) than diesel which implies biodiesel could be a promising directly injected fuel substitute in DFM combustion engines. Some experimental studies have been conducted on DFM combustion engines where biodiesel was used as a pilot fuel. Yoon and Lee [25] compared four combustion conditions include single-fuel (diesel and biodiesel) and dual fuel (biogas/diesel and biogas/biodiesel). Lower NO_x emissions was obtained for DFM compared to single-fuel combustion. In addition, a shortened ignition delay was observed for biogas/biodiesel compared to biogas/diesel due to the higher CN of biodiesel. Ryu [26,27] investigated the effects of pilot injection time and pressure on the combustion and emissions characteristics in a DFM combustion engine. A trade-off between NO_x and smoke was observed for the adjustment on either injection timing or pressure. Furthermore, a numerical study on biodiesel based DFM combustion was done recently. Zhou et al. studied [28] the effects of blend ratio of methanol/biodiesel while maintaining a constant total energy input in DFM combustion using newly developed skeletal reaction mechanism. It was concluded that the increase of methanol could respectively reduce NO_x emissions under 10% load and soot emissions over a wide range of loads significantly.

From the perspective of modelling, the reported numerical studies [4,6,29,30] on gasoline/diesel DFM combustion adopted the primary reference fuel (PRF) mechanism which consists of 41 species and 130 reactions developed by University of Wisconsin-Madison [31]. However, NO_x and soot mechanism are not included. In addition, there is no available mechanism for DFM modelling on gasoline/biodiesel fueled engines. Therefore, a multi-component reaction mechanism, including gasoline, diesel and biodiesel, will be developed for both DFM and BFM combustion in this study. Based on the integrated mechanism, modelling on both gasoline/diesel and gasoline/biodiesel combustion for DFM and BFM are achievable. This paper presents the numerical work based on the developed chemistry mechanism on four combustion scenarios including RCCI fueled by gasoline and diesel, hence discussing the influence of fuel reactivity gradient on combustion process. However, the RCCI combustion fueled by gasoline and biodiesel will be investigated in the future based on this developed chemical reaction mechanism.

2. Reaction mechanism development

2.1. Integration of skeletal mechanism

As mentioned, the objective is to develop a new chemistry mechanism that could model both gasoline/diesel and gasoline/biodiesel combustion for DFM and BFM. Furthermore, the reactions related to NO_x and soot emissions will be embedded in the developed mechanism. Therefore, three mechanisms that have been used to represent the combustion of diesel, biodiesel and gasoline were selected to integrate together.

In this study, *n*-heptane is considered as the surrogate fuel of diesel; hence, the reduced *n*-heptane oxidation chemistry reported by Golovitchev et al. [32], containing 57 species and 217 reactions, was selected for further integration with other mechanisms. Both chemistry mechanism of NO_x and soot emissions have been contained. The reactions that describe the formation of NO_x emissions include Zeldovich mechanism, N_2O to NO branch and NO to NO_2 branch. Considering soot formation, series of elementary reactions lead acetylene and hydrogen to the formation of the first aromatic ring. Then the successive stages of HACA mechanism (H abstraction, C_2H_2 addition) build up a precursor of soot, namely acenaphthylene. Finally, the soot is formed via "graphitization" process $A2R5 \rightarrow 4H_2 + 12C(s)$. The soot model has been applied to predict the soot formation in both diesel and biodiesel combustion [33–35]. Furthermore, considering iso-octane as the surrogate of gasoline, PRF mechanism containing 41 species and 130 reactions reported by Ra and Reitz [31] was selected. In addition, the multi-component mechanism containing 69 species and 204